09/ 836,586

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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 09	JAPIO to be reloaded August 25, 2002
NEWS 20	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 21	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 22	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 23	Aug 26	Sequence searching in REGISTRY enhanced

NEWS EXPRESS	February 1 CURRENT WINDOWS VERSION IS V6.0d, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:41:27 ON 28 AUG 2002

09/ 836,586

=> file reg
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 0.21 | 0.21

FILE 'REGISTRY' ENTERED AT 16:41:36 ON 28 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 26 AUG 2002 HIGHEST RN 444986-65-6
DICTIONARY FILE UPDATES: 26 AUG 2002 HIGHEST RN 444986-65-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

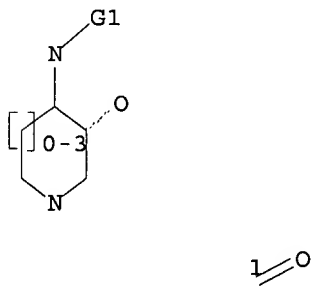
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 09836586.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 CH2,SO2,[@1]

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 16:42:00 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1412 TO ITERATE

70.8% PROCESSED 1000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 25987 TO 30493
PROJECTED ANSWERS: 2884 TO 4514

09/ 836,586

L2 50 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 16:42:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 27559 TO ITERATE

100.0% PROCESSED 27559 ITERATIONS 3406 ANSWERS
SEARCH TIME: 00.00.07

L3 3406 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	140.28	140.49

FILE 'CAPLUS' ENTERED AT 16:42:22 ON 28 AUG 2002
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907 - 28 Aug 2002 VOL 137 ISS 9
FILE LAST UPDATED: 26 Aug 2002 (20020826/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s l3
L4 858 L3

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.19	141.68

FILE 'REGISTRY' ENTERED AT 16:44:05 ON 28 AUG 2002
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STRUCTURE FILE UPDATES: 26 AUG 2002 HIGHEST RN 444986-65-6
DICTIONARY FILE UPDATES: 26 AUG 2002 HIGHEST RN 444986-65-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when

conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

```
=> d his

     (FILE 'HOME' ENTERED AT 16:41:27 ON 28 AUG 2002)

     FILE 'REGISTRY' ENTERED AT 16:41:36 ON 28 AUG 2002
L1             STRUCTURE UPLOADED
L2              50 S L1
L3            3406 S L1 FUL

     FILE 'CAPLUS' ENTERED AT 16:42:22 ON 28 AUG 2002
L4             858 S L3

     FILE 'REGISTRY' ENTERED AT 16:44:05 ON 28 AUG 2002

=> s l3 and leucin?
        119313 LEUCIN?
L5           31 L3 AND LEUCIN?

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       4.38     146.06

FILE 'CAPLUS' ENTERED AT 16:44:37 ON 28 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 28 Aug 2002  VOL 137 ISS 9
FILE LAST UPDATED: 26 Aug 2002  (20020826/ED)
```

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

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=> s l5
L6             5 L5

=> d l6 1- ibib abs hitstr
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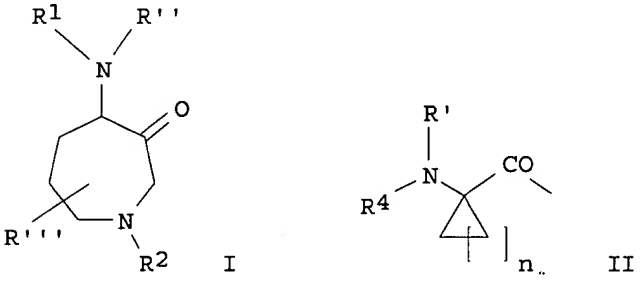
09/ 836,586

YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/(N):y

L6 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:171694 CAPLUS
DOCUMENT NUMBER: 136:232208
TITLE: Preparation of 4-aminoazepan-3-one parasitic cysteine protease inhibitors effective against malaria and other diseases
INVENTOR(S): Tew, David G.; Thompson, Scott K.; Veber, Daniel F.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, UK
SOURCE: PCT Int. Appl., 220 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002017924	A1	20020307	WO 2001-US27178	20010831
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001086983	A5	20020313	AU 2001-86983	20010831

PRIORITY APPLN. INFO.: US 2000-653815 A2 20000901
US 2001-881334 A2 20010614
WO 2001-US27178 W 20010831
OTHER SOURCE(S): MARPAT 136:232208
GI



AB The present invention relates to methods of treating parasitic diseases which are mediated by cysteine proteases by administration of 4-aminoazepan-3-one protease inhibitors I (e.g. benzo[1,3]dioxole-5-carboxylic acid [(S)-1-(1-benzyl-3-oxoazepan-4-ylcarbamoyl)-3-methylbutyl]amide) and pharmaceutically acceptable salts, hydrates and solvates thereof. In particular, the present invention relates to a method of treating malaria by inhibiting the cysteine protease falcipain. Other diseases against which the claimed compds. are effective include trypanosomiasis (African sleeping sickness, Chagas disease), leishmaniasis, schistosomiasis, onchocerciasis (river blindness) and giardiasis. In I: R1 is R4NR'CHR3C(O)-, R5XCHR3C(O)-, R3CH2C(O)-, R4NR'CR''''R3C(O)-, II. R2 is H, C1-6alkyl, C3-6cycloalkyl-C0-6alkyl, Ar-C0-6alkyl, Het-C0-6alkyl, R9C(O)-, R9C(S)-, R9SO2-, R9OC(O)-,

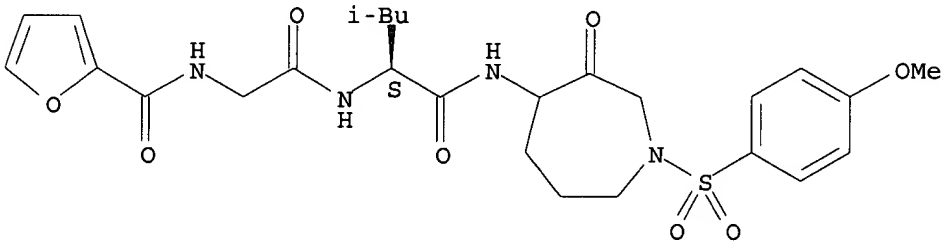
R9R11NC(O)-, R9R11NC(S)-, R9(R11)NSO2-, 3-(2-pyridyl)benzylcarbonyl, 2-(3-(2-pyridyl)phenyl)ethyl, R7NR6CHR8Z-, and R9SO2R11NC(O)-. R3 is H, C1-6alkyl, C3-6cycloalkyl-C0-6alkyl, C2-6alkenyl, C2-6alkynyl, HetC0-6alkyl and ArC0-6alkyl. R3 and R' may be connected to form a pyrrolidine, piperidine or morpholine ring. R4 is H, C1-6alkyl, C3-6cycloalkyl-C0-6alkyl, Ar-C0-6alkyl, Het-C0-6alkyl, R5C(O)-, R5C(S)-, R5SO2-, R5OC(O)-, R5R12NC(O)-, and R5R12NC(S)-. R5 is H, C1-6alkyl, C2-6alkenyl, C2-6alkynyl, C3-6cycloalkyl-C0-6alkyl, Ar-C0-6alkyl and Het-C0-6alkyl. R6 is H, C1-6alkyl, Ar-C0-6alkyl, and Het-C0-6alkyl. R7 is H, C1-6alkyl, C3-6cycloalkyl-C0-6alkyl, Ar-C0-6alkyl, Het-C0-6alkyl, R10C(O)-, R10C(S)-, R10SO2-, R10OC(O)-, R10R13NC(O)-, and R10R13NC(S)-. R8 is H, C1-6alkyl, C2-6alkenyl, C2-6alkynyl, HetC0-6alkyl and ArC0-6alkyl. R9, R10 independently = C1-6alkyl, C3-6cycloalkyl-C0-6alkyl, Ar-C0-6alkyl and Het-C0-6alkyl. R11, R12, R13, R', R'' independently = H, C1-6alkyl, Ar-C0-6alkyl, and Het-C0-6alkyl. R''' is H, C1-6alkyl, C3-6cycloalkyl-C0-6alkyl, Ar-C0-6alkyl, and Het-C0-6alkyl; R'''' is C1-6alkyl, C3-6cycloalkyl-C0-6alkyl C2-6alkenyl, C2-6alkynyl, HetC0-6alkyl and ArC0-6alkyl. X is CH2, S, and O; Z is C(O) and CH2; n is 1-5. Although the methods of prepn. are not claimed, 220 example prepns. are included.

IT **403605-60-7P**, Furan-2-carboxylic acid [[[(1S)-1-[[1-(4-methoxybenzenesulfonyl)-3-oxoazepan-4-yl]carbamoyl]-3-methylbutyl]carbamoyl]methyl]amide **403606-20-2P**, (R)-1-Benzyl-5-oxopyrrolidine-2-carboxylic acid [(1S)-3-methyl-1-[[3-oxo-1-(pyridine-2-sulfonyl)azepan-4-yl]carbamoyl]butyl]amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 4-aminoazepan-3-one parasitic cysteine protease inhibitors effective against malaria and other diseases)

RN 403605-60-7 CAPLUS

CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[hexahydro-1-[(4-methoxyphenyl)sulfonyl]-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

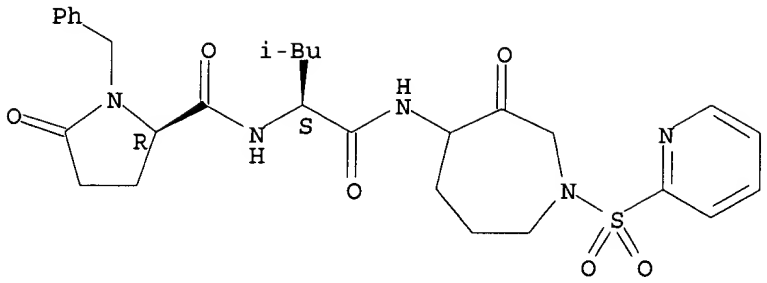
Absolute stereochemistry.



RN 403606-20-2 CAPLUS

CN L-Leucinamide, 5-oxo-1-(phenylmethyl)-D-prolyl-N-[hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



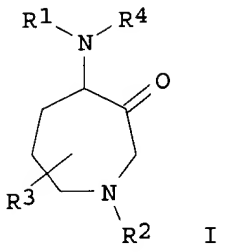
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:923616 CAPLUS
DOCUMENT NUMBER: 136:53691
TITLE: Preparation of 4-amino-azepan-3-one protease inhibitors
INVENTOR(S): Marquis, Robert W., Jr.; Ru, Yu; Veber, Daniel F.; Cummings, Maxwell D.; Thompson, Scott K.; Yamashita, Dennis
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 322 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001095911	A1	20011220	WO 2001-US19062	20010614

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-593845 A2 20000614
OTHER SOURCE(S): MARPAT 136:53691
GI



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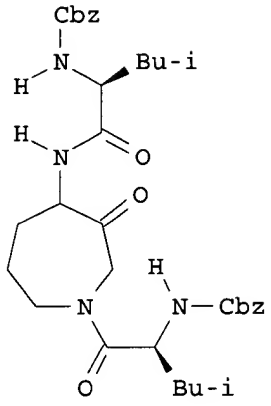


II

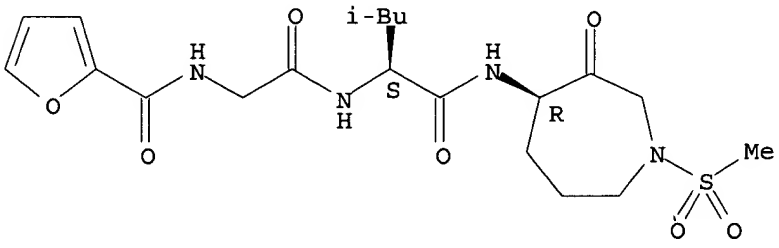
AB The title compds. [I; R1 = COCR13NR11R12, COCR13XR15, COCH2R13; R2 = H, alkyl, cycloalkylalkyl, etc.; R3 = H, alkyl, cycloalkylalkyl, etc.; R4 = H, alkyl, arylalkyl, etc.; R11 = H, alkyl, arylalkyl, etc.; R12 = H, alkyl, cycloalkyl, etc.; R13 = H, alkyl, alkenyl, etc.; R15 = H, alkyl, alkenyl, etc.] which inhibit proteases (no data), including cathepsin K, and are useful for treating diseases of excessive bone loss or cartilage or matrix degrdn. including osteoporosis, gingival disease including gingivitis and periodontitis, arthritis, more specifically, osteoarthritis and rheumatoid arthritis, Paget's disease, hypercalcemia of malignancy, and metabolic bone disease, were prepd. E.g., a multi-step synthesis of compd. II was given.

IT **281215-81-4P 281215-88-1P 281215-94-9P**
281215-99-4P 281216-82-8P 281216-92-0P
281216-93-1P 281217-89-8P 281217-96-7P
281218-02-8P 281218-07-3P 281218-86-8P
281218-95-9P 281218-97-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 4-amino-azepan-3-one protease inhibitors)

RN 281215-81-4 CAPLUS

CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4R)-hexahydro-1-(methylsulfonyl)-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

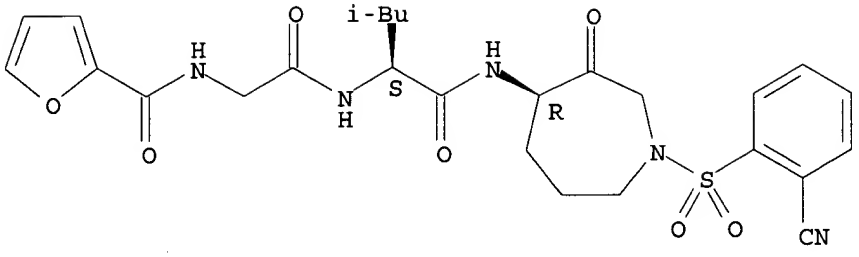
Absolute stereochemistry.



RN 281215-88-1 CAPLUS

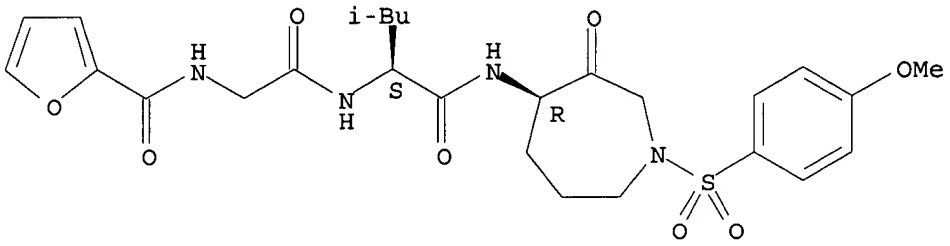
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4R)-1-[(2-cyanophenyl)sulfonyl]hexahydro-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



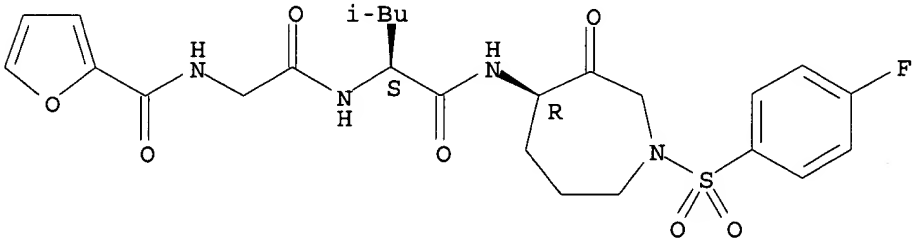
RN 281215-94-9 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4R)-hexahydro-1-[(4-methoxyphenyl)sulfonyl]-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



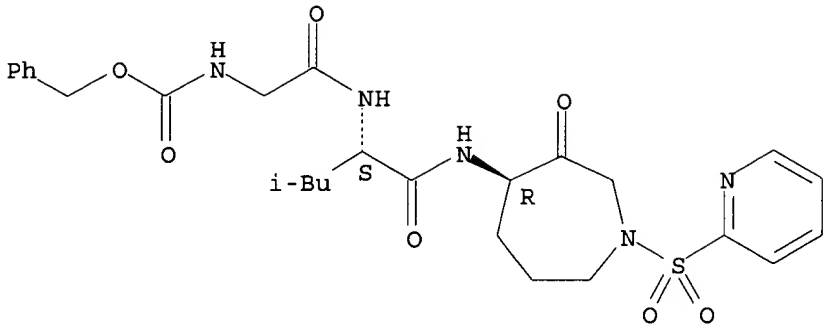
RN 281215-99-4 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4R)-1-[(4-fluorophenyl)sulfonyl]hexahydro-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



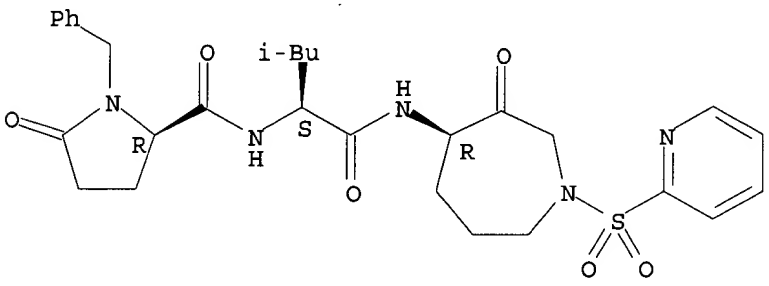
RN 281216-82-8 CAPLUS
CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]glycyl-N-[(4R)-hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



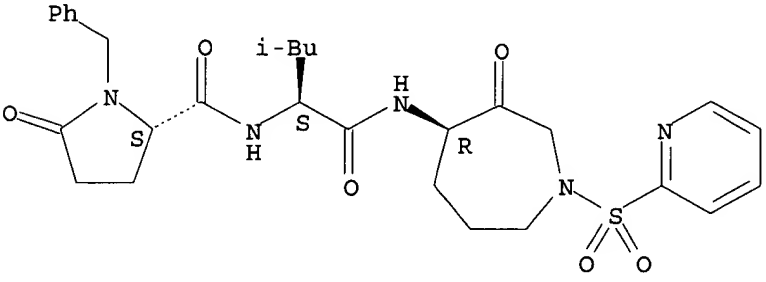
RN 281216-92-0 CAPLUS
CN L-Leucinamide, 5-oxo-1-(phenylmethyl)-D-prolyl-N-[(4R)-hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



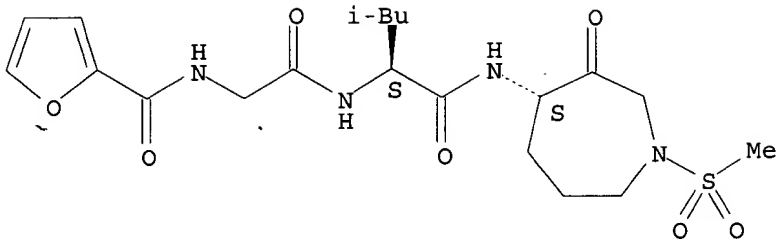
RN 281216-93-1 CAPLUS
CN L-Leucinamide, 5-oxo-1-(phenylmethyl)-L-prolyl-N-[(4R)-hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



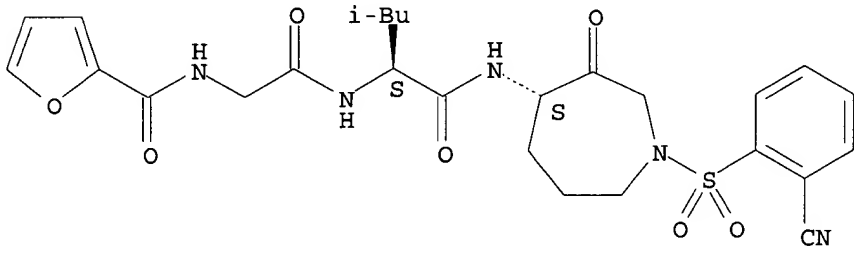
RN 281217-89-8 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4S)-hexahydro-1-(methylsulfonyl)-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



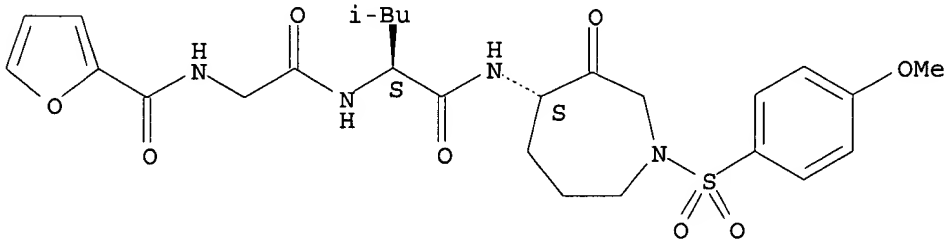
RN 281217-96-7 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4S)-1-[(2-cyanophenyl)sulfonyl]hexahydro-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



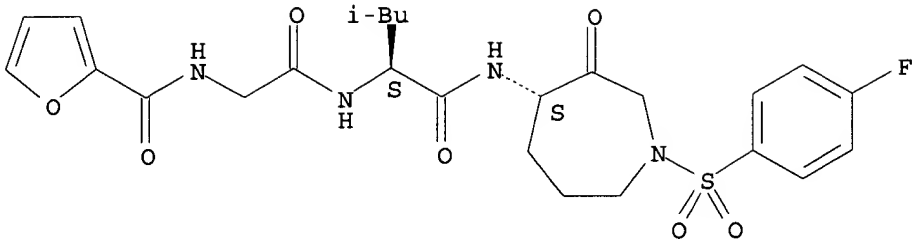
RN 281218-02-8 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4S)-hexahydro-1-[(4-methoxyphenyl)sulfonyl]-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



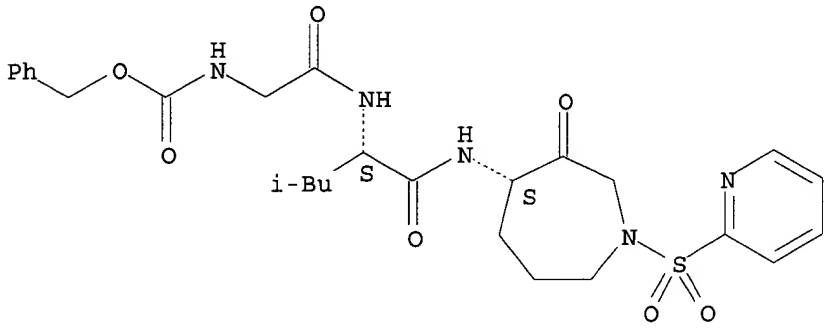
RN 281218-07-3 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4S)-1-[(4-fluorophenyl)sulfonyl]hexahydro-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



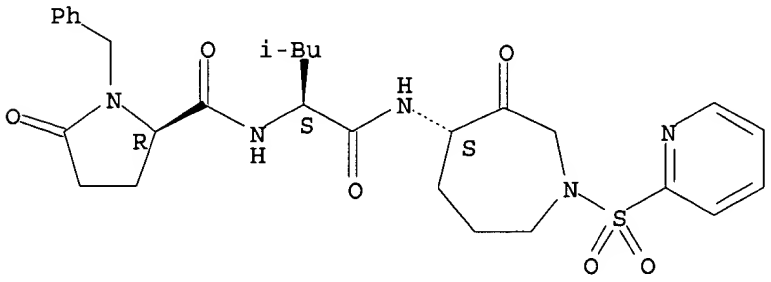
RN 281218-86-8 CAPLUS
CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]glycyl-N-[(4S)-hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



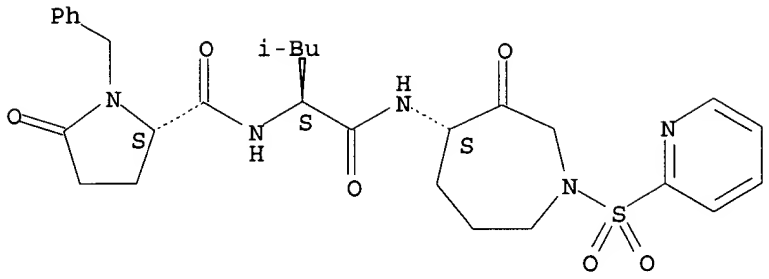
RN 281218-95-9 CAPLUS
CN L-Leucinamide, 5-oxo-1-(phenylmethyl)-D-prolyl-N-[(4S)-hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 281218-97-1 CAPLUS
CN L-Leucinamide, 5-oxo-1-(phenylmethyl)-L-prolyl-N-[(4S)-hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

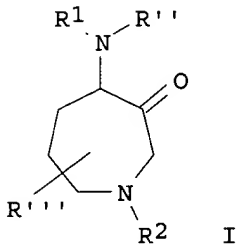
L6 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:713145 CAPLUS
DOCUMENT NUMBER: 135:273219
TITLE: Preparation of C1-6 alkyl-4-aminoazepan-3-one derivatives as protease inhibitors
INVENTOR(S): Cummings, Maxwell D.; Marquis, Robert W., Jr.; Ru, Yu; Thompson, Scott K.; Veber, Daniel F.; Yamashita, Dennis S.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 173 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001070232	A1	20010927	WO 2001-US7094	20010307

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:
US 2000-191000P P 20000321
US 2000-206341P P 20000523
US 2000-211759P P 20000614
US 2000-217445P P 20000710

OTHER SOURCE(S): MARPAT 135:273219
GI



I

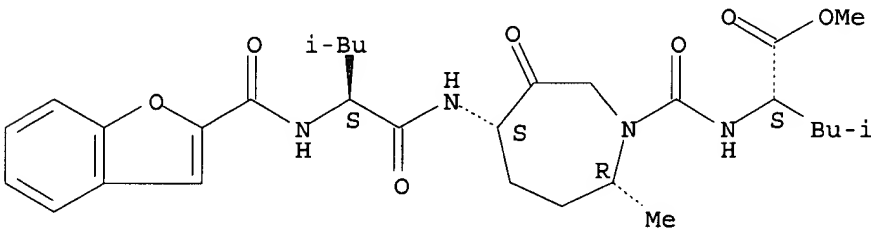
AB 4-Aminoazepan-3-one derivs. I [R1 is an acyl group R3CH2CO, R4NR'CRR3CO or R5-X-CHR3CO; R = H or RR3 = (CH2)n (n = 1-5); R2-R5 = H, alkyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, etc.; R', R'' = H, alkyl, aryl, arylalkyl, heterocyclyl, heterocyclylalkyl; X = CH2, S or O; R''' = alkyl; R3 and R' may be connected to form a pyrrolidine, piperidine or morpholine ring] or their pharmaceutically acceptable salts were prepd. as protease inhibitors for treating various diseases, including excessive bone loss or cartilage or matrix degrdn. Thus, 5-methoxybenzofuran-2-carboxylic acid [(S)-3-methyl-1-[(4S,6S)- (or 4R,6R)-6-methyl-3-oxo-1-(pyridine-2-sulfonyl)azepan-4-ylcarbamoyl]butyl]amide was prepd. by a multistep procedure involving coupling of 4-amino-6-methyl-1-(pyridine-2-sulfonyl)azepan-3-ol (prepn. given) with Boc-Leu-OH and 5-methoxybenzofuran-2-carboxylic acid.

IT **362507-09-3P 362509-05-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of alkyl aminoazepanone derivs. as protease inhibitors)

RN 362507-09-3 CAPLUS

CN L-Leucine, N-(2-benzofuranylcarbonyl)-L-leucyl-(2R,5S)-5-aminohexahydro-2-methyl-6-oxo-1H-azepine-1-carbonyl-, methyl ester (9CI) (CA INDEX NAME)

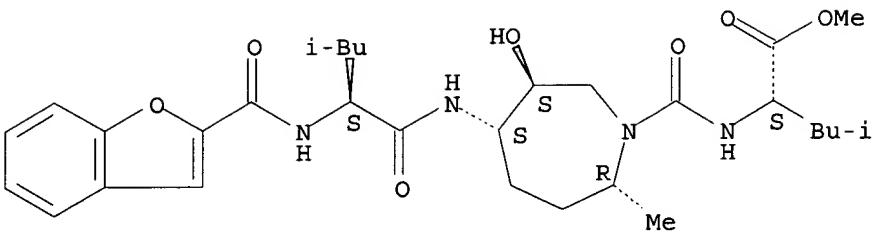
Absolute stereochemistry.



RN 362509-05-5 CAPLUS

CN L-Leucine, N-(2-benzofuranylcarbonyl)-L-leucyl-(2R,5S,6S)-5-aminohexahydro-6-hydroxy-2-methyl-1H-azepine-1-carbonyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

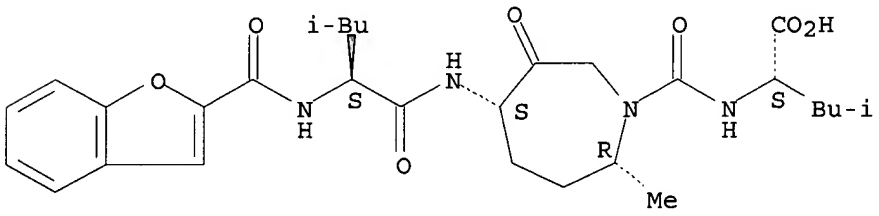


IT **362507-12-8P 362507-15-1P 362507-19-5P**
362507-22-0P 362507-25-3P 362507-28-6P
362507-31-1P 362509-08-8P 362509-11-3P
362509-14-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of alkyl aminoazepanone derivs. as protease inhibitors)

RN 362507-12-8 CAPLUS

CN L-Leucine, N-(2-benzofuranylcarbonyl)-L-leucyl-(2R,5S)-5-aminohexahydro-2-methyl-6-oxo-1H-azepine-1-carbonyl- (9CI) (CA INDEX NAME)

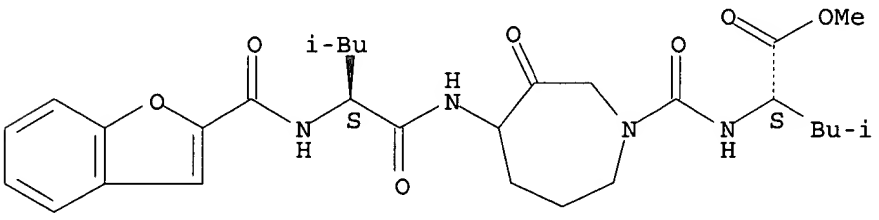
Absolute stereochemistry.



RN 362507-15-1 CAPLUS

CN L-Leucine, N-(2-benzofuranylcarbonyl)-L-leucyl-4-aminohexahydro-3-oxo-1H-azepine-1-carbonyl-, methyl ester (9CI) (CA INDEX NAME)

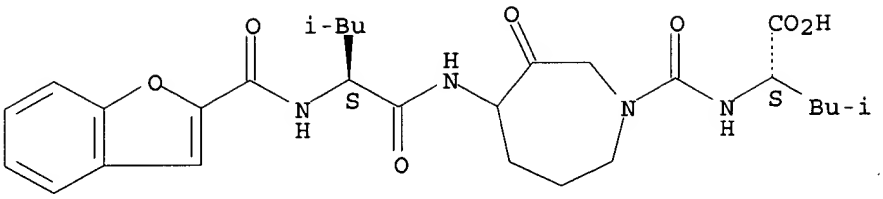
Absolute stereochemistry.



RN 362507-19-5 CAPLUS

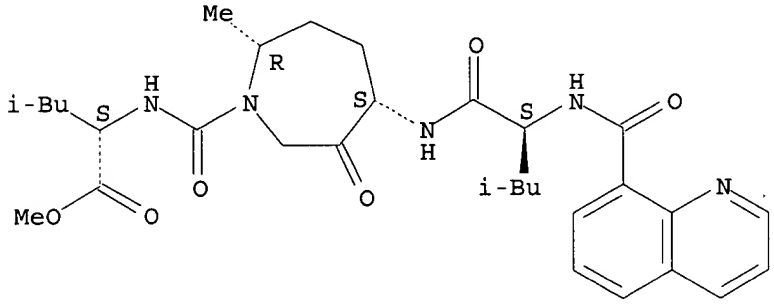
CN L-Leucine, N-(2-benzofuranylcarbonyl)-L-leucyl-4-aminohexahydro-3-oxo-1H-azepine-1-carbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



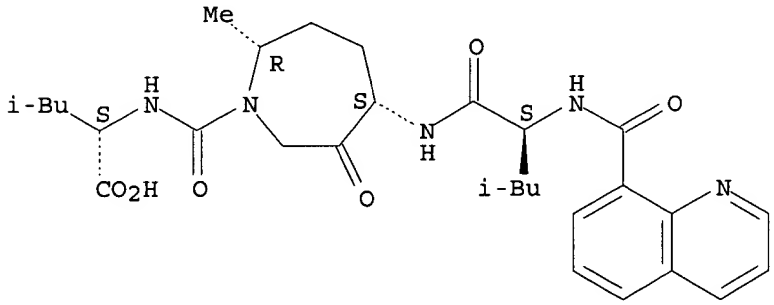
RN 362507-22-0 CAPLUS
CN L-Leucine, N-(8-quinolinylcarbonyl)-L-leucyl-(2R,5S)-5-aminohexahydro-2-methyl-6-oxo-1H-azepine-1-carbonyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



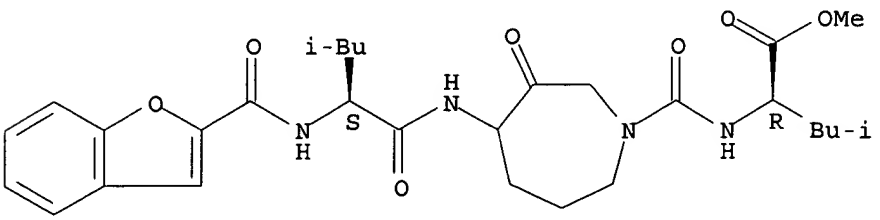
RN 362507-25-3 CAPLUS
CN L-Leucine, N-(8-quinolinylcarbonyl)-L-leucyl-(2R,5S)-5-aminohexahydro-2-methyl-6-oxo-1H-azepine-1-carbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



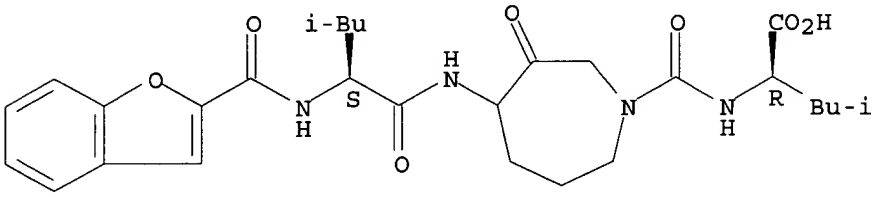
RN 362507-28-6 CAPLUS
CN D-Leucine, N-(2-benzofuranylcarbonyl)-L-leucyl-4-aminohexahydro-3-oxo-1H-azepine-1-carbonyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



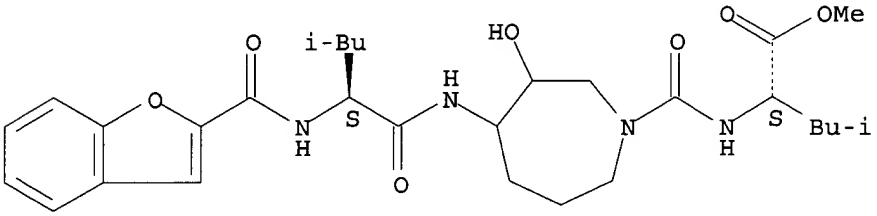
RN 362507-31-1 CAPLUS
CN D-Leucine, N-(2-benzofuranylcarbonyl)-L-leucyl-4-aminohexahydro-3-oxo-1H-azepine-1-carbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



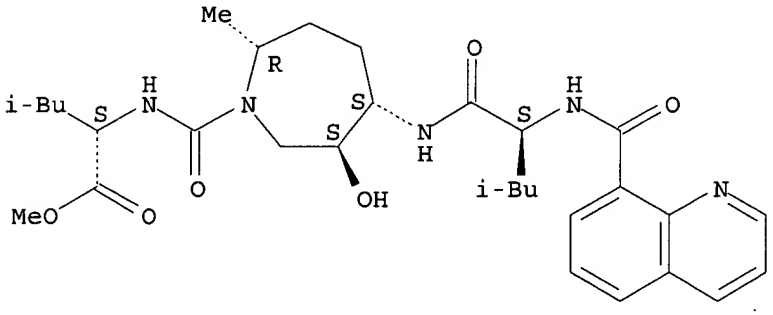
RN 362509-08-8 CAPLUS
CN L-Leucine, N-(2-benzofuranylcarbonyl)-L-leucyl-4-aminohexahydro-3-hydroxy-1H-azepine-1-carbonyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



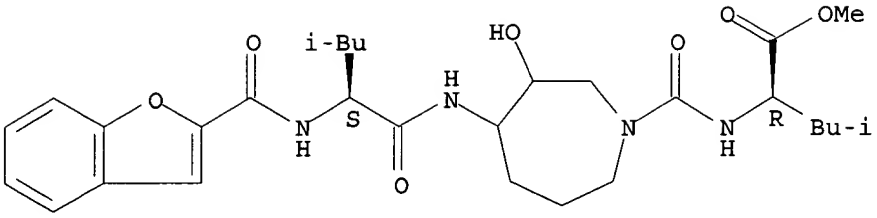
RN 362509-11-3 CAPLUS
CN L-Leucine, N-(8-quinolinylcarbonyl)-L-leucyl-(2R,5S,6S)-5-aminohexahydro-6-hydroxy-2-methyl-1H-azepine-1-carbonyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



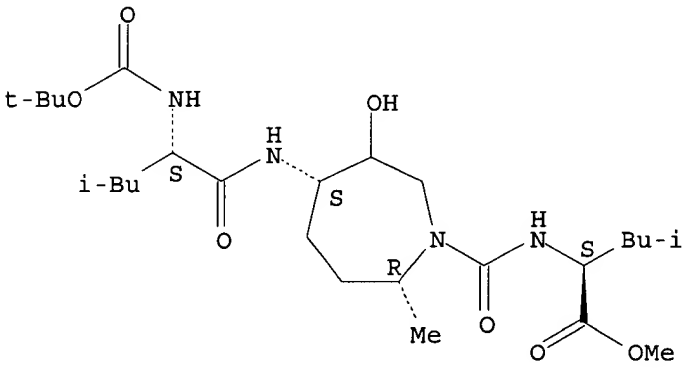
RN 362509-14-6 CAPLUS
CN D-Leucine, N-(2-benzofuranylcarbonyl)-L-leucyl-4-aminohexahydro-3-hydroxy-1H-azepine-1-carbonyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



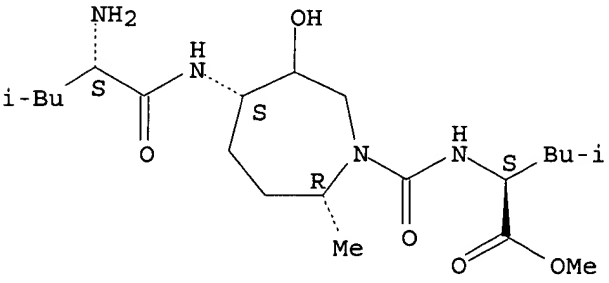
IT **362510-45-0P 362510-47-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of alkyl aminoazepanone derivs. as protease inhibitors)
RN 362510-45-0 CAPLUS
CN L-Leucine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-(2R,5S)-5-aminohexahydro-6-hydroxy-2-methyl-1H-azepine-1-carbonyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 362510-47-2 CAPLUS
CN L-Leucine, L-leucyl-(2R,5S)-5-aminohexahydro-6-hydroxy-2-methyl-1H-azepine-1-carbonyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:456887 CAPLUS
DOCUMENT NUMBER: 133:89444
TITLE: Preparation of 4-amino-azepan-3-one protease inhibitors

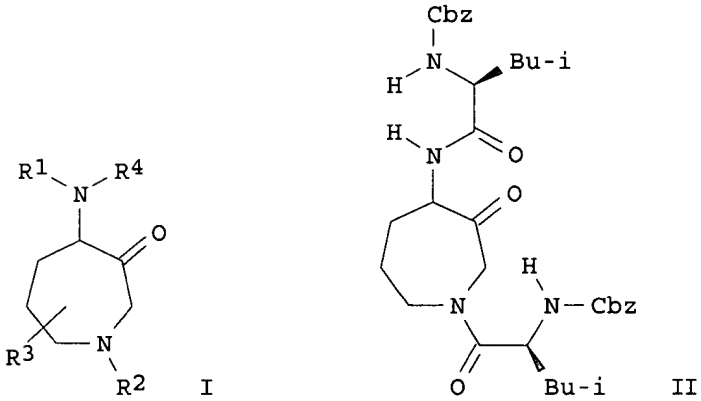
09/ 836,586

INVENTOR(S): Marquis, Robert Wells, Jr.; Ru, Yu; Veber, Daniel Frank; Cummings, Maxwell David; Thompson, Scott Kevin; Yamashita, Dennis
PATENT ASSIGNEE(S): Smithkline Beecham Corp., USA
SOURCE: PCT Int. Appl., 273 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000038687	A1	20000706	WO 1999-US30730	19991221
W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CZ, EE, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 9916488	A	20011009	BR 1999-16488	19991221
EP 1158986	A1	20011205	EP 1999-963112	19991221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
NO 2001003124	A	20010622	NO 2001-3124	20010622

PRIORITY APPLN. INFO.:			
	US 1998-113636P	P	19981223
	US 1999-164581P	P	19991110
	WO 1999-US30730	W	19991221

OTHER SOURCE(S): MARPAT 133:89444
GI

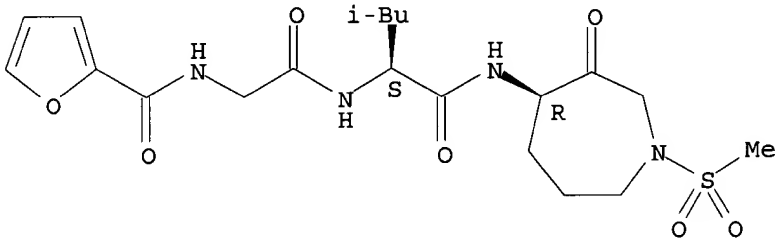


AB The title compds. [I; R1 = COCR13NR11R12, COCR13XR15, COCH2R13; R2 = H, alkyl, cycloalkylalkyl, etc.; R3 = H, alkyl, cycloalkylalkyl, etc.; R4 = H, alkyl, arylalkyl, etc.; R11 = H, alkyl, arylalkyl, etc.; R12 = H, alkyl, cycloalkyl, etc.; R13 = H, alkyl, alkenyl, etc.; R15 = H, alkyl, alkenyl, etc.] which inhibit proteases (no data), including cathepsin K, and are useful for treating diseases of excessive bone loss or cartilage or matrix degrdn. including osteoporosis, gingival disease including gingivitis and periodontitis, arthritis, more specifically, osteoarthritis and rheumatoid arthritis, Paget's disease, hypercalcemia of malignancy, and metabolic bone disease, were prepd. E.g., a multi-step synthesis of compd. II was given. Compds. I are effective at 0.4-400 mg/kg/day.

IT **281215-81-4P 281215-88-1P 281215-94-9P**
281215-99-4P 281216-82-8P 281216-92-0P
281216-93-1P 281217-89-8P 281217-96-7P
281218-02-8P 281218-07-3P 281218-86-8P
281218-95-9P 281218-97-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 4-amino-azepan-3-one protease inhibitors)

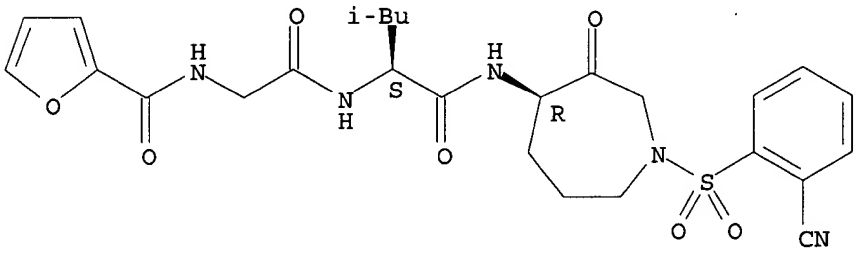
RN 281215-81-4 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4R)-hexahydro-1-(methylsulfonyl)-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



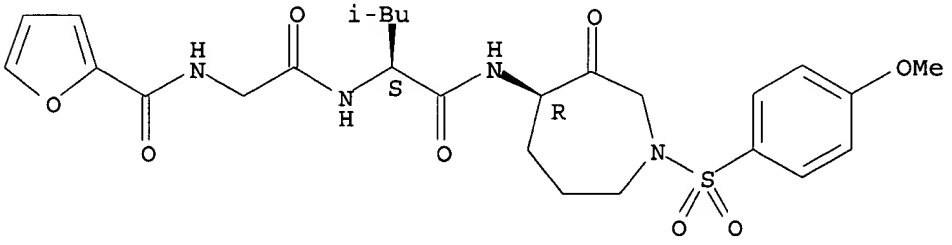
RN 281215-88-1 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4R)-1-[(2-cyanophenyl)sulfonyl]hexahydro-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 281215-94-9 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4R)-hexahydro-1-[(4-methoxyphenyl)sulfonyl]-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

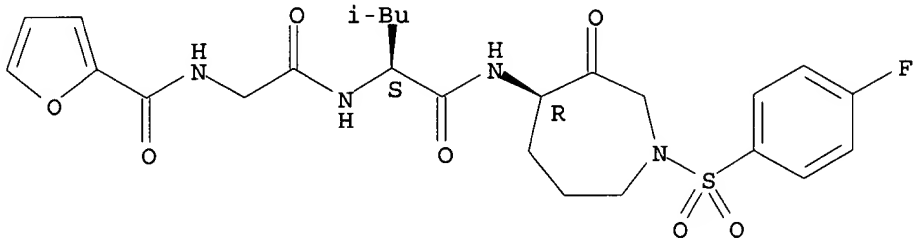
Absolute stereochemistry.



RN 281215-99-4 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4R)-1-[(4-

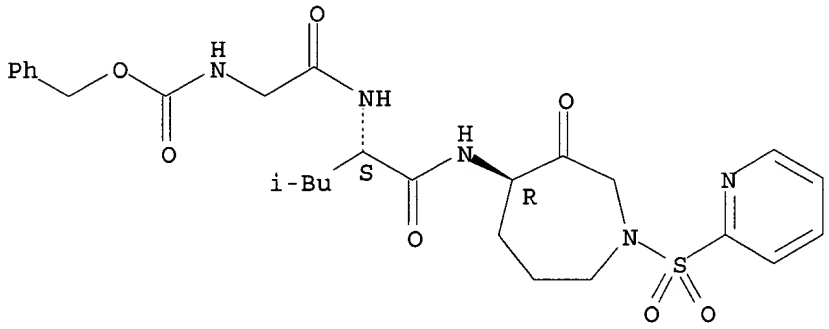
fluorophenyl)sulfonyl]hexahydro-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



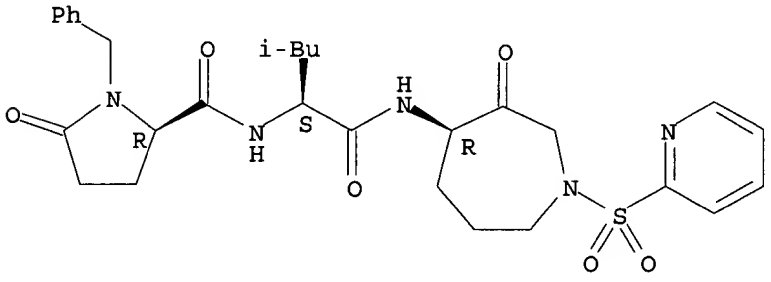
RN 281216-82-8 CAPLUS
CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]glycyl-N-[(4R)-hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



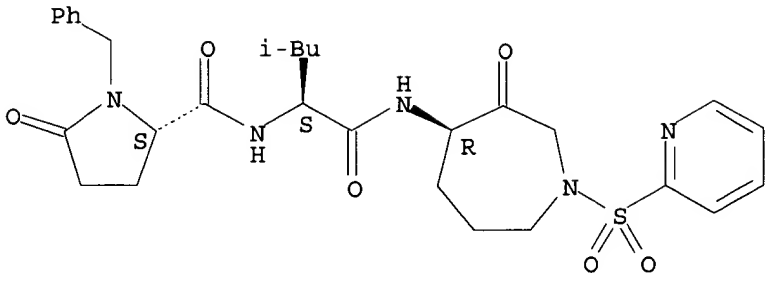
RN 281216-92-0 CAPLUS
CN L-Leucinamide, 5-oxo-1-(phenylmethyl)-D-prolyl-N-[(4R)-hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



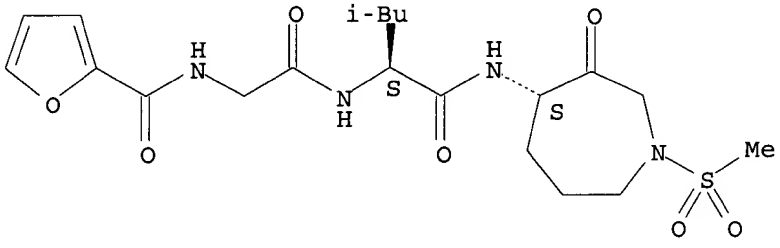
RN 281216-93-1 CAPLUS
CN L-Leucinamide, 5-oxo-1-(phenylmethyl)-L-prolyl-N-[(4R)-hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



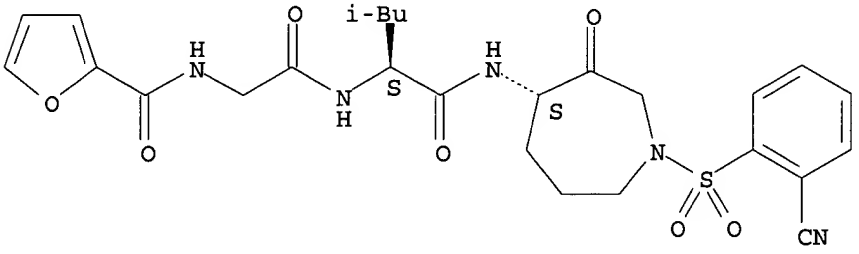
RN 281217-89-8 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4S)-hexahydro-1-(methylsulfonyl)-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



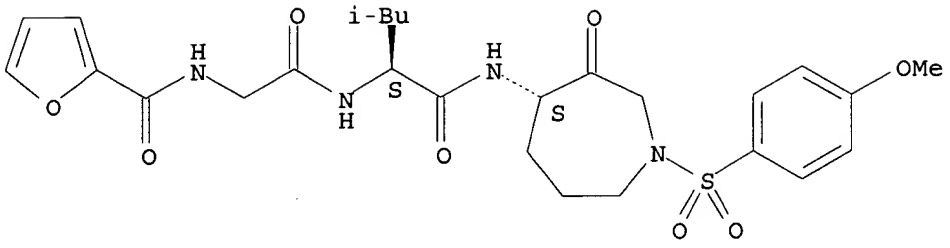
RN 281217-96-7 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4S)-1-[(2-cyanophenyl)sulfonyl]hexahydro-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



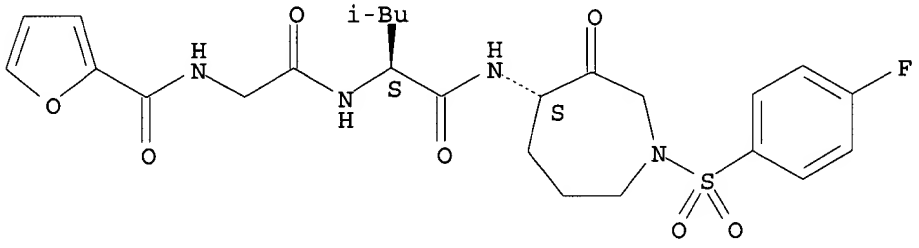
RN 281218-02-8 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4S)-hexahydro-1-[(4-methoxyphenyl)sulfonyl]-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



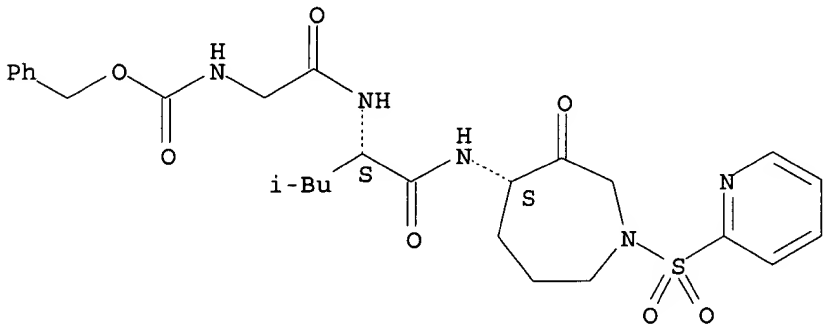
RN 281218-07-3 CAPLUS
CN L-Leucinamide, N-(2-furanylcarbonyl)glycyl-N-[(4S)-1-[(4-fluorophenyl)sulfonyl]hexahydro-3-oxo-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 281218-86-8 CAPLUS
CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]glycyl-N-[(4S)-hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 281218-95-9 CAPLUS
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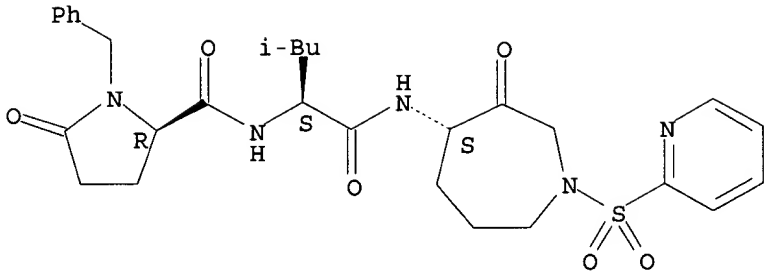
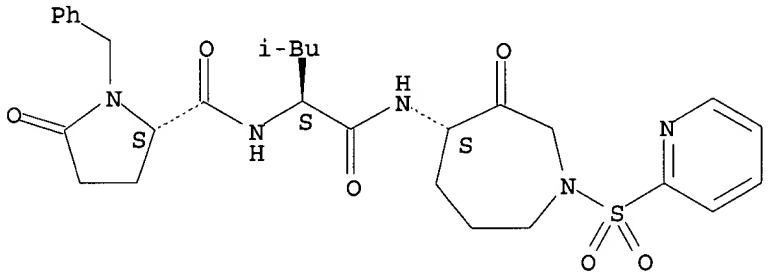
Absolute stereochemistry.



RN 281218-97-1 CAPLUS
CN L-Leucinamide, 5-oxo-1-(phenylmethyl)-L-prolyl-N-[(4S)-hexahydro-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

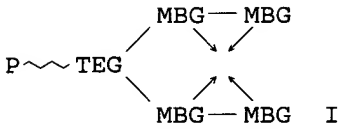
L6 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:197471 CAPLUS
DOCUMENT NUMBER: 128:265374
TITLE: Combinatorial approach for generating novel coordination complexes
INVENTOR(S): Jacobsen, Eric N.; Francis, Matthew B.; Finney, Nathaniel S.
PATENT ASSIGNEE(S): President and Fellows of Harvard College, USA; Jacobsen, Eric N.; Francis, Matthew B.; Finney, Nathaniel S.
SOURCE: PCT Int. Appl., 89 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9812156	A1	19980326	WO 1997-US16740	19970919
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9745851	A1	19980414	AU 1997-45851	19970919

09/ 836,586

PRIORITY APPLN. INFO.: US 1996-26432P P 19960920
WO 1997-US16740 W 19970919

GI



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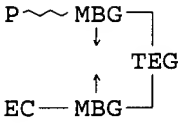


II

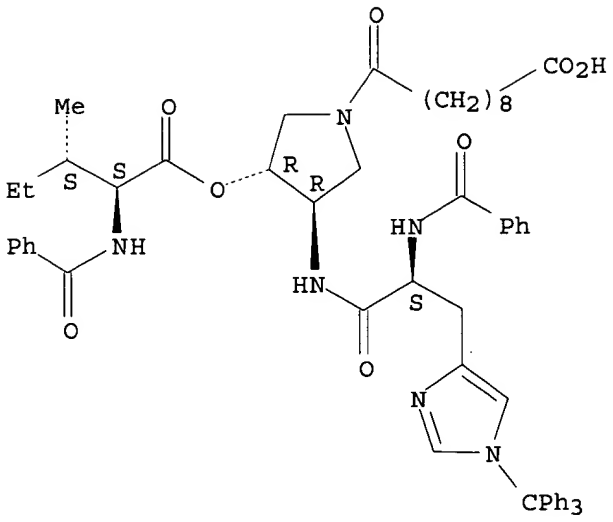
AB The present invention provides methods and compns., i.e. synthetic libraries of binding moieties, for identifying compds. which bind to a metal atom or to non-metal ions, e.g., cationic or anionic mols. Thus, combinatorial libraries, e.g. I and II (P = TentaGel S amino resin polymer support; TEG = turn element group, i.e. di- or trifunctional cyclic amino alc. or cyclic amino acid; MBG = metal binding group, i.e. amino acid residue; EC = end capping group, i.e. acyl residue) were prepd. and examd. for their ability to coordinate transition metal ions. Thus, a 12,000 member combinatorial library P-NHCO(CH2)5NH-A-B-C-D [III; P-NH2 = TentaGel S amino resin polymer; A (position 1) = L- or D-Asp(OCMe3), L- or D-Ser(CMe3), L- or D-Met, L- or D-Tyr(CMe3), L- or D-phenylglycine, His(CPh3), Gly; C (position 2) = L-Asp(OCMe3), L-Ser(CMe3), L-Tyr(CMe3), L-His(CPh3), L-Met, L-Trp, Gly, L-phenylglycine, 4-piperidinecarboxylic acid; B (turn element) = 1-amino-2-carbonyloxycyclopentane stereoisomers, 1-amino-2-carbonyloxycyclohexane stereoisomers, 1-amino-2-carbonyloxyindane stereoisomers, L-Pro, D-pipecolinic acid; D (end cap) = RCO, tosyl, pyroglutamic acid, R = Me, CMe3, 1-naphthyl, CH2CO2Me, 2-pyridyl, 3,4-methylenedioxyphenyl, PhNH] was prepd. using std. solid-phase peptide coupling techniques. Library III was tested for Ni2+ binding affinity by treatment with 2.5 .times. 10-4 M Ni(OAc)2 in MeOH followed by soln. of dimethylglyoxime in MeOH to form a reddish-pink ppt. trapped in the polymer matrix of about 6 of the 24,000 beads. Tag photolysis and anal. allowed the identification of the individual nickel-binding library members.

IT **205325-10-6DP**, amide with TentaGel S resin
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(combinatorial approach for generating novel coordination complexes)

RN 205325-10-6 CAPLUS

CN L-Isoleucine, N-benzoyl-, (3R,4R)-4-[[(2S)-2-(benzoylamino)-1-oxo-3-[1-(triphenylmethyl)-1H-imidazol-4-yl]propyl]amino]-1-(9-carboxy-1-oxononyl)-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L3            3406 S L1 FUL

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L4             858 S L3

     FILE 'REGISTRY' ENTERED AT 16:44:05 ON 28 AUG 2002
L5              31 S L3 AND LEUCIN?

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L6               5 S L5

=> log y
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                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    22.34     168.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    -3.10      -3.10

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